

## **Supplementary Information**

### **Metabolic variability in children's urinary NMR spectroscopic based metabolic phenotypes**

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**SI table 1. T1 correction factor for metabolite quantification**

Compounds/features	Resonance quantified	T1 (sec)
2-hydroxyisobutyrate	1.36 (s)	1.62
3-hydroxyisobutyrate	1.08 (d)	2.09
4-deoxyerythronic acid	1.11 (d)	2.52
4-deoxythreonic acid	1.24 (d)	1.12
Acetate	1.92 (s)	2.97
Alanine	1.48 (d)	1.58
Carnitine	3.23 (s)	1.19
Citrate	2.55 (d)	0.69
Creatine	3.94 (s)	0.96
Creatinine	4.06 (s)	2.07
Dimethylamine	2.72 (s)	3.36
Formate	8.46 (s)	6.03
Glutamine	2.45 (m)	1.28
Glycine	3.57 (s)	2.54
Hippurate	7.55 (t)	2.13
Isoleucine	1.01 (d)	2.06
Lactate	1.33 (d)	1.43
Leucine	0.96 (t)	1.68
Lysine	1.73 (m)	2.57
p-cresol sulfate	2.35 (s)	2.04
Scyllo-inositol	3.36 (s)	5.53
Succinate	2.41 (s)	2.04
Taurine	3.44 (t)	2.14
Trimethylamine	2.87 (s)	1.72
Trimethylamine oxide	3.27 (s)	1.82
TSP	0(s)	2.69
Valine	1.05 (d)	2.28

**SI Table 2 Univariate analyses of urinary metabolite differences between morning and night-time spot samples.** Bolded values are significant ( $p\text{-value} < 0.0011$ , based on bonferroni correction for 44 tests) based on the Wilcox test. Fold change was calculated as the difference between morning and night concentrations concentration divided by the morning concentration. The median of the fold changes is presented across all individuals.

	Morning/Night			
	Fold change (median %)	p-values	Interquartile range	
2-hydroxyisobutyrate	0%	5.5E-01	-0.22 - 0.19	
3-aminoisobutyrate	-5%	7.4E-01	-0.89 - 0.51	
3-hydroxybutyrate/3-aminoisobutyrate	-8%	9.3E-02	-0.37 - 0.14	
3-hydroxyisobutyrate	-24%	2.6E-02	-0.43 - 0.092	
3-hydroxyisovalerate	-5%	6.5E-01	-0.27 - 0.2	
3-indoxylsulfate	0%	5.8E-01	-0.59 - 0.44	
4-deoxyerythronic acid	4%	5.0E-02	-0.13 - 0.33	
4-deoxythreonic acid	<b>23%</b>	<b>1.3E-06</b>	<b>0.0047 - 0.39</b>	
5-oxoproline	-11%	<b>5.4E-04</b>	<b>-0.32 - 0.03</b>	
Acetate	-36%	<b>3.1E-08</b>	<b>-1 - -0.013</b>	
Acetone	-7%	2.3E-01	-0.95 - 0.37	
Alanine	-17%	<b>8.0E-04</b>	<b>-0.65 - 0.091</b>	
Carnitine	-41%	<b>1.2E-03</b>	<b>-1.6 - 0.27</b>	
Citrate	-52%	<b>8.3E-09</b>	<b>-1.1 - -0.14</b>	
Creatine	-27%	2.1E-02	-1 - 0.18	
Creatinine	14%	9.0E-02	-0.18 - 0.33	
Dimethylamine	3%	3.9E-01	-0.2 - 0.25	
Formate	-31%	<b>5.3E-04</b>	<b>-0.87 - 0.14</b>	
Glucose	-10%	<b>9.2E-03</b>	<b>-0.35 - 0.099</b>	
Glutamine	-7%	6.3E-02	-0.33 - 0.15	
Glycine	-12%	4.7E-02	-0.64 - 0.23	
Hippurate	10%	5.2E-01	-0.53 - 0.36	
Isoleucine	-11%	6.6E-02	-0.41 - 0.17	
Lactate	-9%	3.5E-02	-0.54 - 0.16	
Leucine	-4%	5.3E-01	-0.29 - 0.19	
Lysine	6%	6.7E-01	-0.37 - 0.38	
N <sup>1</sup> -methyl-nicotinamide	<b>53%</b>	<b>3.2E-19</b>	<b>0.25 - 0.71</b>	
N-acetyl neuraminic acid	9%	1.1E-01	-0.091 - 0.18	
N-methyl nicotinic acid	-19%	3.4E-02	-1.5 - 0.38	
N-methyl-2-pyridone-5-carboxamide	<b>23%</b>	<b>1.1E-03</b>	<b>-0.15 - 0.49</b>	
N-methylpicolinic acid	-83%	1.2E-01	-Inf - 0.92	
Panthothentic acid	-20%	<b>6.9E-05</b>	<b>-0.39 - 0.026</b>	
P-cresol sulfate	1%	8.3E-01	-0.55 - 0.36	
p-hydroxyphenylacetate	-24%	<b>2.3E-04</b>	<b>-0.9 - 0.12</b>	
Proline betaine	-1%	7.8E-01	-1.7 - 0.7	
Scyllo-inositol	-12%	4.0E-02	-0.44 - 0.14	
Succinate	-41%	<b>1.7E-05</b>	<b>-1.3 - 0.098</b>	

<b>Sucrose</b>	<b>-148%</b>	<b>5.3E-12</b>	<b>-5.8 - -0.15</b>
Taurine	<b>-36%</b>	<b>3.7E-05</b>	<b>-1.2 - 0.19</b>
<b>Trimethylamine</b>	<b>3%</b>	<b>6.1E-01</b>	<b>-0.11 - 0.18</b>
<b>Trimethylamine oxide</b>	<b>-17%</b>	<b>6.0E-02</b>	<b>-0.9 - 0.39</b>
<b>Tyrosine</b>	<b>-5%</b>	<b>1.4E-01</b>	<b>-0.43 - 0.17</b>
Urea	<b>-12%</b>	<b>5.0E-02</b>	<b>-0.58 - 0.2</b>
<b>Valine</b>	<b>-5%</b>	<b>2.2E-01</b>	<b>-0.3 - 0.16</b>

**SI Table 3 Univariate analyses of urinary metabolite differences between male and female children.** Bolded values are significant ( $p\text{-value} < 0.0011$ , based on bonferroni correction for 44 tests) based on the Wilcox test. Fold change was calculated as the difference between the median male and median female concentration divided by the median male concentration. The median was calculated across all individuals.

	Male/Female	
	Fold change (median %)	p-values
<b>2-hydroxyisobutyrate</b>	<b>53%</b>	<b>1.4E-01</b>
<b>3-aminoisobutyrate</b>	<b>43%</b>	<b>6.5E-15</b>
<b>3-hydroxybutyrate/3-aminoisobutyrate</b>	<b>40%</b>	<b>5.3E-16</b>
<b>3-hydroxyisobutyrate</b>	<b>38%</b>	<b>1.6E-20</b>
<b>3-hydroxyisovalerate</b>	<b>38%</b>	<b>1.7E-07</b>
<b>3-indoxylsulfate</b>	<b>37%</b>	<b>7.3E-05</b>
<b>4-deoxyerythronic acid</b>	<b>35%</b>	<b>2.0E-08</b>
<b>4-deoxythreonic acid</b>	<b>33%</b>	<b>4.2E-08</b>
<b>5-oxoproline</b>	<b>30%</b>	<b>1.1E-05</b>
<b>Acetate</b>	<b>30%</b>	<b>6.1E-14</b>
<b>Acetone</b>	<b>28%</b>	<b>5.9E-12</b>
<b>Alanine</b>	<b>26%</b>	<b>1.7E-11</b>
<b>Carnitine</b>	<b>25%</b>	<b>1.4E-10</b>
<b>Citrate</b>	<b>24%</b>	<b>1.7E-07</b>
<b>Creatine</b>	<b>22%</b>	<b>5.8E-06</b>
<b>Creatinine</b>	<b>21%</b>	<b>3.8E-12</b>
<b>Dimethylamine</b>	<b>19%</b>	<b>7.5E-07</b>
<b>Formate</b>	<b>19%</b>	<b>3.0E-02</b>
<b>Glucose</b>	<b>18%</b>	<b>4.9E-09</b>
<b>Glutamine</b>	<b>18%</b>	<b>5.1E-04</b>
<b>Glycine</b>	<b>17%</b>	<b>6.9E-06</b>
<b>Hippurate</b>	<b>17%</b>	<b>3.6E-02</b>
<b>Isoleucine</b>	<b>17%</b>	<b>3.0E-05</b>
<b>Lactate</b>	<b>14%</b>	<b>3.9E-04</b>
<b>Leucine</b>	<b>14%</b>	<b>3.5E-08</b>
<b>Lysine</b>	<b>14%</b>	<b>1.7E-09</b>
<b>N<sup>1</sup>-methyl-nicotinamide</b>	<b>13%</b>	<b>5.4E-02</b>
<b>N-acetyl neuraminic acid</b>	<b>12%</b>	<b>8.4E-04</b>
<b>N-methyl nicotinic acid</b>	<b>12%</b>	<b>4.3E-07</b>

N-methyl-2-pyridone-5-carboxamide	11%	3.0E-03
N-methylpicolinic acid	11%	9.9E-02
Pantotenic acid	8%	3.0E-01
P-cresol sulfate	7%	3.4E-01
p-hydroxyphenylacetate	7%	7.6E-01
Proline betaine	5%	6.3E-01
<i>Scyllo</i> -inositol	5%	6.3E-01
Succinate	4%	8.3E-01
Sucrose	2%	2.1E-01
Taurine	1%	4.1E-04
Trimethylamine	-1%	9.1E-01
Trimethylamine oxide	-2%	7.4E-01
Tyrosine	-13%	5.4E-01
Urea	-14%	2.2E-02
Valine	-20%	5.6E-04

**SI Table 4 Diurnal metabolic variation in urine samples (N=108 pairs first morning and night-time samples) across 6 consecutive days in 20 children aged 8-9 yrs old.** The ratios represent the difference between the morning and night samples divided by the mean of the two samples. Colours are associated with the direction of the metabolite concentration difference, higher concentration in morning samples are in green, lower in red.

Day/ Child	1	2	3	4	5	6	1	2	3	4	5	6	1	2	3	4	5	6	1	2	3	4	5	6
	Acetate						Acetone						Alanine						Carnitine					
1	-0.08		-0.22	-0.01	-1.00	-0.03	-0.38		0.04	0.12	0.50	0.06	0.03		-0.06	-0.32	-0.45	0.58	-0.84		0.01	-1.40	-1.11	0.14
2	-0.54	-0.91		0.00	0.89	-0.20	-0.20	-1.41		0.72	-0.44	-0.14	0.13	0.38		-0.38	0.21	-0.03	1.03	1.60		-1.37	0.98	0.24
3	-0.28	0.31	-1.37	0.28	-0.87	0.33	-0.70	-0.49	-0.37	-0.35	0.22	0.82	-0.12	0.38	-0.25	0.29	-0.16	-0.57	-1.64	-0.47	0.92	-1.84	0.58	-1.71
4	0.17	0.31	1.11	-0.21		-0.50	0.66	0.08	0.88	-0.66		-0.17	0.06	-0.41	0.64	-0.26		0.19	0.40	1.01	0.25	-0.40		0.65
5	-0.16	-0.66	-0.54	-0.83	-0.43	-0.43	0.47	-0.52	-0.43	-0.66	-0.65	-2.00	-0.69	-0.30	0.10	-1.08	-0.30	-0.40	-0.94	0.23	-1.00	-0.73	0.03	-0.40
6		-0.03	-0.34	-0.37	-0.55	0.27		0.43	-0.50	-0.18	-0.24	0.11		0.03	-0.14	0.33	-0.47	0.17		-0.41	-0.26	-1.83	0.20	0.06
7	0.32		-0.12	-0.59	-0.88	-0.05	0.28		-1.45	-0.13	2.00	0.09	0.00		-0.37	-0.40	-1.01	-0.50	0.82		0.57	-1.44	-1.33	0.61
8	-0.01	-0.52	0.57	-0.11	-0.12	-0.45	-1.76	0.31	-1.60	0.19	0.20	0.42	1.23	-0.55	0.78	-0.70	0.37	-0.71	0.75	-1.09	1.00	-0.20	1.39	-1.32
9	-0.80	0.28	-0.86	0.77	-0.47	-1.36	-0.45	1.14	-1.21	-0.64	0.70	0.45	-0.43	0.49	0.13	0.94	-0.58	0.02	0.85	1.08	-0.89	-0.52	-0.93	-0.17
10		0.29	-0.21	-0.14	0.28	-0.10		-0.02	-0.55	-0.29	0.50	-0.06		0.52	-1.03	0.05	0.63	-0.49		-0.59	0.46	-0.22	-0.20	-0.62
11	-0.15	-0.47	-0.42	-0.77	0.05	-0.07	-0.30	-0.33	-1.64	-1.16	-0.99	-0.37	0.64	0.08	0.04	-0.40	-0.28	-0.17	0.27	0.12	-1.51	-0.69	-1.93	-0.67
12	-0.12	-0.37	0.05	0.06	-0.25	-1.03	0.44	-0.72	0.46	-0.29	0.04	0.46	0.59	0.32	-0.27	0.02	0.09	-0.27	0.90	-0.45	-1.22	0.09	0.29	0.84
13	-0.35	0.06	0.19	-0.39	-0.39	-0.77	-1.72	-0.61	0.81	-0.77	-1.16	0.74	-0.12	0.19	-0.43	-0.09	-0.15	-0.58	-0.22	-0.39	-0.14	-0.06	-0.47	-1.12
14	-0.17	-0.51		2.00	-1.11	-0.99	0.21	-0.54		0.41	2.00	-2.00	0.10	-0.36		-0.14	-0.72	-0.85	1.08	0.15		-0.96	-1.35	-0.47
15	0.17	-0.18	0.22	-0.16	-1.43	-0.33	-0.55	0.78	-0.11	0.43	0.73	0.51	0.10	-0.63	0.17	-0.11	-0.30	-0.99	-0.46	1.10	-0.70	-0.56	0.92	-0.88
16	-1.42	-0.50			-0.38	-0.61	-1.18	-0.67		1.13	-0.38	-0.87	-0.83				-0.13	-0.86	-0.20	-0.89			-0.22	-0.74
17	1.29	0.40	-0.12		-0.73	-0.25	1.26	0.59	0.53		0.23	-0.76	0.52	-0.19	-0.87		-1.14	-0.16	0.57	0.47	-0.94		-0.44	0.45
18	-0.01	-1.11	-0.22	-1.60	-1.35	-0.27	0.14	-0.80	-1.34	-1.67	0.89	-1.06	-0.44	-1.05	0.09	-0.76	-1.47	-0.32	-0.57	-0.71	0.64	-1.78	-1.35	-0.86
19		-1.15		-1.15	-0.65	-0.66		-1.54		-0.23	0.29	0.95		-0.20		-1.37	-0.15	0.05		0.40		-0.88	-1.45	-0.17
20	-0.74	-0.78	-1.00	-0.86	-0.16	-0.84	-0.92	1.09	0.73	1.19	0.54	-0.41	-0.34	-0.68	-1.25	-0.87	0.52	-0.31	-0.23	-1.46	-1.29	-0.69	0.03	-1.28
	Citrate						Creatine						Creatinine						Dimethylamine					
1	-0.31		-0.14	-0.51	-0.78	0.37	-0.26		0.10	0.01	-0.06	0.39	0.29		0.40	0.01	-0.06	-0.04	0.36		0.18	-0.12	-0.08	0.26
2	-0.36	-0.43		0.18	0.18	-0.11	0.04	-0.05		0.05	-0.54	-0.53	-0.08	0.97		-0.44	-0.90	0.13	-0.11	0.69		0.39	0.34	0.11
3	-0.73	-0.32	-0.43	-0.22	-0.18	0.30	-0.03	0.89	1.15	0.21	0.85	-1.79	0.49	-0.15	1.36	0.22	0.14	-0.83	0.48	-0.05	-0.25	0.04	-0.14	-0.15

	Metabolite A										Metabolite B										Metabolite C									
	Formate	Glucose	Glutamine	Glycine	Formate	Glucose	Glutamine	Glycine	Formate	Glucose	Glutamine	Glycine	Formate	Glucose	Glutamine	Glycine	Formate	Glucose	Glutamine	Glycine										
1	0.16	-0.02	-0.25	-0.82	0.34	0.07	-0.30	0.06	-0.65	0.32	0.04	0.29	-0.31	-0.16	0.64	0.25	0.17	-0.45	-0.30	0.59										
2	0.23	-0.79	-0.03	0.94	-0.10	0.03	0.17	-	-0.34	0.08	-0.02	0.19	0.09	-	0.00	0.45	0.23	0.17	0.33	-	0.01	0.25	0.37							
3	-0.51	-0.08	-0.88	0.32	-0.90	-0.10	0.06	-0.39	-0.27	0.00	-0.06	-0.50	0.26	0.29	-0.93	0.79	-0.75	-0.22	-0.06	0.31	-0.36	0.38	-0.18	-0.49						
4	0.60	-0.01	1.11	-0.02	-	0.66	0.36	-0.08	0.18	0.09	-	-0.23	0.51	-0.02	0.50	-0.28	-	0.15	0.56	-0.15	1.03	-0.36	-	-0.09						
5	-0.32	-0.55	0.35	-1.50	-0.01	-0.19	0.24	-0.53	0.02	-0.63	-0.44	-0.02	-0.10	-0.05	0.04	-0.28	-0.47	-0.11	-0.41	0.05	-0.05	-0.93	-0.23	-0.30						
6	-	0.17	-0.09	0.05	-0.47	0.30	-	0.06	-0.06	0.01	-0.13	-0.05	-	0.19	-0.37	-0.11	-0.32	-0.24	-	0.13	-0.32	0.16	-0.50	0.37						
7	-0.08	-	-0.50	0.02	-0.63	0.23	0.55	-	-0.15	0.17	-0.32	-0.30	0.04	-	0.09	0.23	-0.23	-0.02	0.19	-	-0.41	-0.32	-0.69	0.37						
8	1.14	-0.79	0.57	-0.56	0.27	-1.10	-0.08	-0.07	-0.26	0.38	-0.16	-0.08	0.20	-0.62	0.66	-0.20	0.32	-0.08	1.05	-0.48	1.14	-0.49	0.45	-0.90						
9	-0.46	0.19	-0.31	0.91	-0.19	-0.63	0.09	0.01	-0.01	0.26	0.40	-0.39	0.13	0.12	-0.11	0.46	0.02	0.20	0.09	0.07	-0.10	0.75	-0.35	0.19						
10	-	0.73	-0.89	0.00	0.45	-0.56	-	0.36	-0.35	-0.04	0.16	-0.08	-	0.23	-0.52	-0.28	0.24	-0.10	-	0.70	-0.64	0.12	0.73	-0.31						
11	-0.14	-0.53	-0.74	-1.07	-0.45	-1.08	0.25	0.34	0.03	-0.09	0.28	-0.21	0.22	-0.13	0.06	-1.20	-0.21	0.10	0.37	0.04	-0.26	-0.72	0.48	-0.03						

12	-0.17	-0.08	-0.58	0.02	-0.36	-0.60	-0.19	-0.37	0.19	0.14	0.01	-0.21	0.37	-0.33	-0.30	-0.06	-0.17	0.22	0.54	0.30	-0.46	0.33	-0.22	-0.03
13	-0.29	0.18	-0.08	0.16	-0.32	-0.80	-0.45	0.43	0.41	-0.10	-0.52	0.13	-0.20	-0.14	0.10	-0.04	0.29	-0.01	-0.21	0.04	0.08	-0.27	-0.62	-0.74
14	0.15	1.30		0.31	-1.29	-1.21	-0.43	-0.27		-0.23	-0.98	-0.37	0.20	-0.40		0.45	-0.67	-0.94	0.20	-0.42		0.35	-0.81	-0.82
15	0.15	-0.45	0.35	-0.44	-0.90	-0.51	-0.05	-0.50	-0.06	0.30	-0.19	0.00	-0.16	0.03	-0.07	0.09	-0.04	-0.18	0.40	0.17	0.17	-0.55	0.38	-1.14
16	-0.90	-1.19			-2.00	-1.29	-0.16	-0.22		-0.46	-0.33	-1.05	-0.51			-0.11	-0.50	-1.11	-0.59			-0.19	-0.79	
17	1.00	0.09	-0.20		-1.01	-0.09	0.01	0.22	-0.04	-0.90	0.16	0.89	-0.01	-0.51		-0.99	0.22	1.00	0.31	-0.80		-1.05	0.13	
18	-0.07	-0.53	0.09	-1.07	-1.55	-0.34	-0.10	-0.74	0.19	0.04	-0.64	-0.40	-0.34	-0.27	-0.04	-1.25	-0.78	-0.27	0.16	-0.92	-0.28	-1.04	-1.14	-0.64
19		0.14		-1.64	-0.09	-0.59		-0.01		-0.63	0.19	-0.01		-0.21		-0.70	-0.30	0.11		0.01		-1.19	-0.27	0.26
20	0.24	-1.03	-1.55	-0.59	0.03	-0.34	0.35	-0.05	-0.40	-0.39	-0.07	0.28	-0.19	-0.09	-0.41	-0.24	0.16	-0.53	-0.07	-0.49	-0.91	-1.04	0.54	-0.78
Hippurate						N-methylpicolinic acid						Isoleucine						Lactate						
1	-0.23		0.41	0.15	0.28	-0.61	1.63			-0.60	-0.02	-1.71	-0.13		0.09	-0.29	-0.33	0.63	0.32		0.20	-0.40	-0.12	0.56
2	0.62	0.40		0.66	0.51	-0.26	0.32	1.48		1.71	2.00	-2.00	0.51	-0.88		0.15	0.41	0.35	0.14	-0.14		0.23	0.35	0.22
3	-0.44	1.32	-0.75	-0.36	0.04	0.38	1.09	-2.00	-2.00	-2.00	-2.00	2.00	-0.01	0.82	0.18	0.43	-0.19	0.16	-0.15	0.14	-0.18	0.15	0.05	-0.22
4	0.34	-0.35	-0.07	0.33		-0.74	N	2.00	-1.99	1.78		-0.99	0.40	0.09	0.48	0.19		0.08	0.64	0.05	1.05	-0.42		0.15
5	0.95	-0.31	0.06	0.53	-0.49	0.74	0.99	-2.00	-2.00	-1.56	2.00	-2.00	0.23	-0.18	-0.39	-0.37	-0.43	-0.19	-0.16	-0.05	-0.12	-0.76	-0.35	-0.23
6		-0.05	-0.37	-0.39	0.16	-0.08		-2.00	-2.00		-0.61	-2.00		0.35	-0.28	0.06	0.18	0.19		0.07	-0.10	0.14	-0.37	0.20
7	-0.60		1.16	0.76	0.59	-0.67	2.00		2.00	-2.00	0.77	-1.98	0.06		-0.19	-0.57	-0.23	-0.26	-0.04		-0.41	-0.20	-0.59	0.26
8	-0.21	-0.48	0.40	-1.32	1.71	-1.58	-2.00	1.34	-0.54	2.00	1.95	1.43	-0.84	0.20	0.27	0.35	0.49	-1.15	0.57	-0.36	0.89	-0.47	-0.05	-0.71
9	-0.99	0.18	-0.27	-0.16	1.34	-1.22	1.23		2.00	1.12	-0.65	2.00	-0.42	0.57	-0.62	-0.42	0.17	-0.84	-0.05	0.55	-0.36	1.10	-0.44	0.50
10		1.70	0.32	-0.32	-0.31	0.62		2.00	-2.00		2.00			0.25	0.03	0.18	0.17	0.18	0.64	-0.65	0.10	0.65	-0.33	
11	-1.23	1.39	-0.38	0.33	0.86	-0.05	2.00	2.00	-2.00		-2.00	-2.00	-0.12	-0.11	-0.54	-0.47	-0.50	0.16	0.50	0.10	-0.10	-0.94	0.04	0.16
12	-0.06	-0.45	0.38	0.55	-0.29	-0.41	-2.00		-2.00	-1.52	-2.00	-0.76	0.45	-0.48	-0.15	0.00	0.55	-0.19	0.49	0.14	-0.33	0.14	0.10	-0.09
13	1.01	-0.65	-1.10	-0.08	-1.08	1.21	-2.00	1.03	0.64	-1.51	-1.94	1.88	-0.44	0.31	0.12	0.19	-0.51	-0.31	-0.30	0.39	0.20	-0.55	0.20	-0.50
14	0.00	-0.41		-0.47	0.06	-0.43	-2.00	-1.97		1.04		-1.96	0.07	-0.57		0.10	-0.28	-0.83	0.31	-0.43		-0.07	-0.82	-0.88
15	-0.37	-0.25	-0.51	0.25	-1.32	0.00	-2.00	0.55	2.00	2.00	-2.00	1.67	-0.15	-0.30	-0.54	-0.74	-0.30	-0.02	0.05	0.08	0.09	-0.58	0.57	-0.80
16	0.08	0.67			0.03	-0.35	0.15	-0.90		-2.00			-0.07	-0.50				-0.09	-0.16	-0.61	-0.76		-0.06	-0.58
17	-0.60	0.16	0.19		-1.66	0.97	-2.00	2.00	0.31		-1.75	-2.00	0.51	0.61	-0.07		-0.49	0.08	0.73	0.24	-0.53		-0.61	-0.29
18	-0.44	0.19	-0.74	1.36	-0.19	0.44	2.00	0.66		-0.30	2.00		0.07	-0.50	0.25	-0.39	-0.13	0.25	-0.14	-0.98	-0.25	-0.60	-1.23	-0.39
19	0.19		-0.44	0.17	0.90		-2.00		-2.00	1.58	-1.81		0.71		-0.59	0.08	0.14		-0.81		-1.04	-0.29	-0.02	

20	0.44	0.79	0.00	1.59	-0.59	0.62	-1.74	N	2.00	N	2.00	-0.71	-0.21	0.07	-0.15	-0.02	0.18	-0.38	-0.45	-0.28	-0.72	-0.85	0.42	-0.39						
	<b>Leucine</b>						<b>Lysine</b>						<b>N-acetyl neuraminic acid</b>						<b>N-methyl-2-pyridone-5-carboxamide</b>											
1	0.01		0.08	-0.28	0.24	0.40	0.64		0.53	-0.14	0.44	1.16	0.15		0.01	-0.04	0.08	0.16	0.29		1.68	0.38	-0.41	0.60						
2	0.18	0.14		-0.10	0.30	0.32	0.12	0.10		0.07	0.17	0.46	0.21	-0.02		-0.48	0.09	0.03	-0.01	0.48		1.28	0.65	0.41						
3	0.20	0.28	0.12	1.11	-0.77	-0.55	-0.73	0.66	0.27	0.19	0.96	-0.17	-0.42	-0.56	-0.59	0.02	-0.11	-0.17	-0.40	0.71	0.63	-0.08	-0.36	0.70						
4	0.56	-0.02	0.64	0.00		-0.06	0.61	-0.12	0.62	-0.11		-0.87	0.09	-0.10	0.11	0.31		0.20	0.64	0.42	0.74	0.20		0.26						
5	0.12	-0.28	0.08	-0.35	-0.19	-0.01	0.07	-0.29	-0.70	0.30	0.07	0.08	0.25	0.12	-0.08	-0.09	0.14	-0.07	0.66	-0.52	0.60	0.12	-0.33	1.09						
6		-0.01	-0.17	0.19	-0.06	0.11		0.13	-0.25	0.47	-0.08	0.22		0.25	0.23	0.07	0.37	0.00	-0.24	0.52	0.74	0.20	0.03							
7	0.13		-0.15	0.24	-0.34	0.46	0.03		-0.60	-0.01	-0.82	0.73	0.70		0.11	-0.45	0.35	-0.53	N		0.35	0.46	0.48	1.02						
8	0.20	-0.32	0.57	0.00	0.40	-0.55	0.93	-0.67	0.90	0.05	-0.18	0.42	-0.34	0.10	0.17	0.18	-0.02	0.14	0.39	-0.08	0.53	1.35	0.72	-0.10						
9	-0.35	0.43	-0.28	-0.19	0.25	0.09	-0.10	0.51	0.05	1.22	-0.17	0.50	-0.29	0.32	0.04	0.00	0.12	0.14	-2.00	-0.33	-0.02	0.41	0.97	0.24						
10		-0.18	-0.25	0.26	0.32	-0.03		1.07	-1.08	0.15	0.49	-0.59		0.11	-0.09	0.14	-0.01	0.26		0.40	-0.01	-0.48	-0.58	-0.60						
11	0.16	0.27	-0.20	-0.57	-0.30	0.29	0.67	0.19	-0.26	-1.02	0.31	0.06	0.27	0.54	0.00	0.25	0.12	0.03	0.28	0.54	-0.27	-0.11	0.66	-0.04						
12	0.52	-0.09	-0.08	0.12	0.24	-0.23	0.96	0.64	-0.30	-0.72	0.62	0.52	-0.04	-0.53	0.28	-0.08	0.20	0.12	0.28	-0.42	0.71	0.33	0.28	-0.23						
13	-0.06	0.18	0.35	0.35	0.06	-0.23	-0.32	0.44	0.46	0.04	0.48	-0.26	0.09	0.02	0.06	0.12	-0.17	0.40	-1.11	0.44	1.35	-0.67	0.31	0.55						
14	0.10	-0.19		0.20	-0.41	-0.13	0.75	-0.23		0.41	-0.63	-0.93	-0.12	-0.31		0.01	0.35	0.13	0.82	-0.51		-2.00	0.37	1.73						
15	0.07	0.17	-0.12	-0.29	0.45	-0.24	0.27	0.37	0.11	-0.73	0.75	-0.63	-0.18	-0.02	0.01	0.77	-0.10	-0.33	-0.37	1.17	-1.27	-0.48	0.11	0.88						
16	-0.92	-0.26			-0.11	-0.29	-0.25	-0.44			0.55	-0.36	-0.03	0.23			-0.20	0.31	1.17	0.02		2.00	0.12							
17	0.12	-0.01	-0.23			-0.36	-0.53	0.56	0.31	-0.31		-0.37	0.11	-0.26	-0.35	0.67		-0.66	-0.03	1.26	0.38	0.04		1.01	-0.17					
18	0.11	-0.58	-0.38	-0.43	-0.52	-0.27	0.40	-0.20	-0.51	-0.80	-0.66	-0.31	-0.36	-0.49	0.12	0.02	0.09	-0.26	0.99	0.54	-1.01	-0.23	1.35	-0.22						
19		0.28		-0.69	-0.17	0.34		0.06		-1.10	0.14	-0.14		0.33		-0.13	0.32	0.06	0.72		0.48	0.63	0.31							
20	0.27	-0.24	-0.44	-0.48	0.34	-0.26		-0.56	-0.44	-0.59	-0.22	0.76	-0.39		0.42	0.27	0.17	0.24	0.53	0.34	-1.46	0.15	0.13	0.01	-1.81	0.00				
	<b>N-Methyl nicotinic acid</b>						<b>N<sup>1</sup>-Methyl-nicotimide</b>						<b>P-cresol sulfate</b>						<b>p-hydroxyphenylacetate</b>											
1	0.10		0.06	-0.26	-0.61	-0.08	0.59		0.67	1.41	0.67	-0.02	1.04		-0.37	0.95	-1.05	1.32	0.07		0.14	0.47	-0.40	0.28						
2	0.03	0.46		0.48	-1.67	-0.07	0.91	-0.03		1.19	1.29	0.83	-0.31	0.32		0.02	0.56	-0.19	0.79	1.24		-0.26	-0.77	-1.05						
3	0.82	-0.94	-0.81	1.00	-0.05	-1.43	0.64	0.81	0.94	0.25	0.84	0.66	-0.32	-0.15	-0.32	0.53	-0.30	0.44	0.19	-0.43	0.44	-0.17	-0.73	-0.60						
4	0.95	-0.32	0.79	0.17		-1.12	0.50	0.61	0.73	0.24		0.56	0.25	-0.09	-0.43	0.97		-0.85	0.80	-1.24	-1.41	0.56		-0.44						
5	-0.82	-0.15	-0.59	-0.54	-0.06	0.61	1.07	0.47	-0.19	0.77	0.09	1.26	0.13	0.21	0.58	0.82	0.43		-0.56	-0.68	0.84	-0.84	-0.47	0.59						
6		-0.71	0.42	0.38	-0.95	-0.44								0.49	0.40	-0.69	0.21	-0.32							-0.39	-0.55	-0.12	0.05	-0.74	

	7	-1.69	-1.59	1.25	-0.28	-1.17	0.49	0.49	0.17	1.29	0.60	-0.61	0.09	-0.43	-0.64	-1.18	-0.02	-0.11	0.13	-0.83	-0.58				
	8	-0.53	-0.84	-1.14	-0.43	-1.11	0.16	-0.08	0.19	0.51	1.69	-0.83	-0.26	0.57	0.27	1.15	-0.16	1.83	-0.40	0.14	-0.99	0.01	0.30	0.22	-0.88
	9	-0.37	-0.40	0.69	1.91	0.99	-0.39	0.56	0.23	0.90	1.01	0.80	0.69	-0.78	-0.72	0.77	-0.71	1.59	-0.43	-1.29	0.98	-0.62	-1.43	0.25	-0.30
	10	1.56	-1.37	-1.30	1.34	-1.23		1.19	1.14	0.14	0.22	-0.51		0.30	0.36	0.37	-0.29	0.37		0.40	-0.12	0.08	-0.25	-0.18	
	11	-0.88	1.00	-0.17	-0.95	0.31	-0.45	0.70	0.78	0.79	0.82	1.31	0.86	-0.36	0.61	-0.42	0.16	0.08	0.43	0.32	0.35	0.61	0.09	0.14	-0.55
	12	-1.35	-1.26	-0.96	0.88	0.75	-0.92	0.60	-0.19	1.41	0.72	0.91	1.70	-1.05	-0.41	0.43	-1.21	0.05	-0.14	0.17	-1.05	0.39	-0.62	0.14	-0.03
	13	0.01	-0.83	1.00	-0.22	-1.44	0.75	0.30	1.20	1.30	0.63	1.16	1.42	-0.24	-0.28	0.13	0.13	-0.26	0.88	-0.64	-0.05	0.03	-0.23	-0.60	0.42
	14	-0.08	-1.19		-0.85	0.73	-0.19	1.31	0.82		0.48	1.10	1.43	-0.05	-0.44		-0.35	-0.27	0.19	-0.41	-0.27		-0.24	-1.42	0.84
	15	0.40	-0.06	-0.75	-0.42	-0.52	-0.17	-0.80	0.04	0.39	0.23	1.15	1.36	-0.14	0.14	-0.04	0.82	0.05	-0.99	-0.52	-0.21	-0.87	-0.11	-1.50	-0.01
	16	-0.40	-1.22			0.75	-0.53	0.82	-0.18			1.22	0.89	-0.13	0.36			0.58	-0.68	-1.35	-0.13			-0.03	-1.04
	17	-1.67	0.62	0.44		-0.46	0.08	1.69	0.77	1.34		1.89	1.09	-0.33	0.62	-0.02		0.01	0.46	-0.33	0.21	0.11		-0.34	0.01
	18	1.12	-1.36	-0.38	-1.20	0.97	0.58	0.55	0.74	-0.04	1.51	1.95	0.81	-0.02	0.03	-0.69	0.49	-0.82	1.65	-0.63	-0.57	-0.43	-0.19	-1.05	-0.89
	19		-0.24		-1.50	1.25	-0.07		0.35		0.41	-0.12	0.65		-0.49		0.91	0.00	-0.48		-0.24		-0.99	0.45	-0.59
	20	0.45	-0.47	0.79	-0.45	1.44	0.57	-0.54	0.39	1.29	-0.43	-0.06	0.85	-0.74	-0.50	1.10	0.64	1.63	-1.63	0.08	-0.40	-0.74	0.34	-0.02	-0.73
	Pantotenic acid					Proline betaine					5-oxoproline					Scyllo-inositol									
1	0.19		0.01	-0.05	-0.09	-0.22	-1.29		-1.30	1.29	0.37	-1.23	-0.11		0.07	-0.05	-0.56	0.34	-0.20		2.00	-2.00	-2.00	-2.00	
2	-0.09	-0.18		0.13	0.04	0.03	-0.94	-0.91		0.27	-0.25	-1.24	0.06	-0.23		-0.14	0.46	-0.04	-0.01	-0.21		0.03	-0.01	-0.13	
3	-0.22	-0.11	-0.46	0.01	-0.29	-0.18	0.00	2.00	0.97	0.42	-2.00	-1.95	-0.09	0.07	-0.56	0.17	-0.31	-0.26	0.08	-0.17	0.54	0.14	-0.23	0.71	
4	0.01	-0.17	0.47	-0.20		0.03	0.10	-1.28	-0.85	-0.40		-1.05	0.50	0.03	0.22	0.04		-0.40	0.42	-0.80	0.07	0.13		-0.32	
5	-0.08	-0.48	-0.38	-0.52	-0.58	-0.01	-0.40	0.84	-1.42	-1.12	1.08	-1.33	-0.30	-0.66	-0.17	-0.27	-0.52	-0.08	-0.03	0.03	-0.65	-0.65	0.22	-0.42	
6		0.03	-0.39	-0.17	0.01	-0.13		-2.00	-2.00	1.26	2.00	0.97		0.00	-0.05	-0.15	0.04	-0.18		0.26	-0.03	-0.07	0.42	-0.02	
7	-0.21		-0.48	-0.03	-0.27	-0.15	-0.43		2.00	-0.42	-1.73	1.32	0.31		-0.25	0.06	-0.62	-0.24	-1.26		-0.72	-0.30	-0.38	-0.09	
8	-0.10	-0.01	0.05	-0.43	0.49	-0.73	-0.01	-0.22	0.30	-0.07	-0.37	-0.72	-0.49	-0.13	-0.17	0.00	-0.28	-0.46	-0.07	-0.18	0.15	0.94	-0.21	-0.60	
9	-0.39	-0.01	-0.38	-0.56	-0.27	-0.14	-0.34	1.55	-1.58	1.27	1.79	1.94	-0.30	-0.08	0.32	0.32	-0.10	-0.27	-0.21	0.16	-0.07	-0.25	-2.00	-0.25	
10		0.47	-0.35	0.03	0.12	0.04		0.82	0.41	1.56	-0.79	-0.19		0.29	-0.03	-0.08	-0.08	0.07		0.37	-0.35	-0.17	0.03	0.15	
11	-0.30	-0.44	0.48	-0.41	0.33	-0.04	0.73	-0.88	-0.02	-0.92	1.08	-0.82	-0.08	0.07	-0.28	-0.11	0.37	-0.34	-0.94	-0.26	0.27	-0.11	-0.33	0.15	
12	0.31	-0.09	-0.01	0.11	-0.06	0.16	-2.00	2.00	-0.66	-1.19	1.88	-0.29	0.08	-0.53	0.08	0.13	-0.15	-0.25	-0.03	2.00	-0.04	0.03	0.37	0.10	
13	-0.42	-0.01	0.02	-0.29	0.19	-0.45	0.69	-2.00	1.87	0.29	0.86	-1.05	-0.08	-0.22	0.06	-2.00	-0.37	-0.11	-0.20	0.42	0.18	0.55	-0.35	0.18	
14	-0.28	-0.56		0.08	-0.24	-0.61	0.21	-0.47		0.45	1.14	-1.53	-0.27	-0.32		0.43	-0.12	-0.09	-0.13	-0.42		0.21	-0.26	-0.06	

15	-0.47	0.12	0.23	0.43	-0.19	-0.49	2.00	0.39	-2.00	2.00	2.00	-0.55	-0.07	-0.05	-0.98	0.21	-0.10	0.01	0.03	-2.00	-2.00	-0.62	0.71	-1.11	
16	-0.16	0.08			-0.02	-0.14	-2.00	0.66		2.00	-1.83		-0.56	-0.20		-0.34	-0.30		-0.78	-0.20			-0.11	-0.60	
17	0.40	-0.16	0.02		-0.63	-0.23	0.21	1.60	N		0.18	0.62	0.57	-0.04	-0.27		-0.99	-0.01	0.61	0.21	-2.00		2.00	-0.11	
18	0.07	-0.68	-0.18	-0.71	-0.32	-0.23	0.81	-0.21	2.00	0.09	1.22	-0.51	-0.19	-0.33	-0.21	-0.47	-0.13	-0.16	-1.37	-0.28	-0.39	0.45	-2.00	-0.71	
19		0.24		-0.40	-0.30	0.45		2.00		-2.00	2.00	-2.00		0.01		-0.43	0.01	0.07		0.47		-0.47	-2.00	-0.23	
20	-0.23	0.02	-0.47	-0.79	-0.04	-0.23	1.28	0.63	-0.04	-2.00	0.82	2.00	-0.04	0.32	-0.21	-0.33	-0.05	-0.10	0.09	0.36	-0.29	-0.14	0.61	-0.22	
Succinate						Sucrose						Taurine						Trimethylamine							
1	0.24		0.07	-0.12	-0.91	0.58	-1.30		-1.89	-0.81	-1.63	0.14	-0.59		-0.47	-0.51	0.40	0.74	-0.20		-0.02	0.35	-0.22	0.51	
2	N		-2.00		-0.15	0.69	-0.23	-1.81	0.16		-1.91	-0.05	-0.68	-0.16	-0.77		-0.44	-0.49	-0.80	0.03	-0.06		-0.03	-0.21	0.26
3	-0.48	-0.37	-1.71	-0.16	-2.00	0.10	-1.06	-1.50	-0.52	-0.99	0.08	-0.71	-0.47	0.34	-1.39	1.19	-0.65	-0.88	0.20	-0.03	-0.05	0.30	-0.02	-0.20	
4	0.33	0.04	2.00	0.21		-0.80	-1.75	0.14	-0.60	-1.52		2.00	-0.16	-1.11	-0.33	0.27		-0.54	0.50	-0.18	0.07	0.23		-0.40	
5	-0.27	-0.71	-0.91	-2.00	-2.00	-2.00	-1.71	-1.97	-1.35	-1.07	-0.76	-1.49	0.57	0.68	0.19	-1.64	-1.61	-1.21	0.42	-0.07	-0.06	-0.10	-0.03	0.15	
6		0.92	-0.25	-0.67	0.69	-0.29		0.38	-0.82	-1.14	-1.96	-0.04		-0.32	-0.34	0.12	-0.11	0.16		0.08	0.17	0.34	0.02	0.25	
7	-0.27		-0.56	0.18	-1.15	0.68	-0.61		0.63	-2.00	-0.52	-1.66	-2.00		0.09	-1.71	-0.95	-1.33	0.09		-0.17	0.18	0.31	-0.73	
8	-0.41	-0.26	0.76	0.68	-0.68	-0.41	0.05	-1.86	-0.53	-0.70	-0.25	0.54	0.35	-0.57	0.42	-0.38	-0.22	2.00	-0.09	0.32	0.08	0.01	-0.08	-0.44	
9	-0.73	-0.27	-0.45	0.97	-0.83	-1.24	-2.00	0.13	0.02	-1.18	-2.00	-0.76	-0.41	-0.11	-0.33	-0.05	-0.14	0.41	-0.06	0.07	-0.17	0.42	-0.08	-0.20	
10		0.56	0.21	0.40	0.88	-0.18		-1.68	-1.24	-1.30	-0.31	-2.00		-0.83	-0.28	0.28	2.00	-0.32		0.55	-0.31	0.24	-0.12	0.00	
11	-0.61	-2.00	-2.00	-0.74	0.55	-0.42	1.13	-0.24	1.19	0.07	-0.46	-0.07	0.56	-0.99	-0.50	-0.22	-0.30	1.30	0.06	0.21	-0.02	-0.03	0.13	-0.17	
12	-0.55	-0.56	-0.16	0.88	-0.33	-1.16	-0.99	-0.16	-1.37	0.36	-0.80	-2.00	0.32	-0.45	0.45	0.09	-0.52	-0.25	0.22	-0.20	0.25	-0.05	0.10	0.09	
13	-2.00	-0.58	0.51	-0.28	-0.79	-0.50	-0.32	0.58	-1.83	-0.47	0.09	-0.09	-1.19	0.13	-0.03	-0.21	-0.75	-0.35	0.06	0.11	0.07	0.20	-0.40	0.05	
14	0.09	-0.50		1.66	-0.91	-1.76	-1.20	-0.82		-1.09	-0.36	-0.87	1.91	-1.65		0.74	-0.89	-1.48	-0.04	-0.88		0.49	-0.07	0.14	
15	0.12	-0.50	-0.21	0.19	-1.19	-0.18	-0.36	-0.90	-0.24	1.16	-1.97	-0.26	-0.46	-0.09	-0.52	-0.50	0.45	0.90	-0.14	0.34	-0.28	-0.05	0.13	0.11	
16	-2.00	-0.91			-1.53	-0.51	-0.79	-0.80			-0.44	-0.39	-0.42	-0.97			0.09	-0.26	-0.08	0.20			0.01	0.00	
17	1.64	-0.28	0.10		-0.70	-2.00	-1.33	0.65	-1.45		-1.69	-0.22	0.54	-0.77	0.69		1.05	0.22	0.15	0.13	0.54		-0.18	0.29	
18	-0.02	-0.71	-2.00	-2.00	-0.21	-0.39	-1.00	-1.98	-0.63	-0.51	-1.72	-0.58	-0.04	-0.75	-0.82	-1.23	-1.14	0.41	0.53	-0.30	-0.40	-0.76	0.01	0.32	
19		-1.17		-0.68	-0.36	0.11		0.97		-1.88	-1.37	0.36		-1.16		-1.16	-0.72	-0.11		0.62		-0.67	0.48	-0.19	
20	-0.61	-0.46	-0.54	2.00	-0.07	-1.21	1.21	-2.00	-0.85	-1.81	-1.81	0.44		-0.16	-0.50	0.40	-0.18	-0.74	-0.10	-0.07	0.00	-0.47	0.57	0.23	
Trimethylamine oxide						Tyrosine						Urea						Valine							
1	1.53		1.36	0.51	-1.01	0.93	-0.06		-0.34	-0.04	-0.14	0.26	-0.31		-0.35	-0.25	-0.18	0.04	0.02		-0.06	-0.20	0.11	0.07	

	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	2-hydroxyisobutyrate	3-aminoisobutyrate	3-hydroxybutyrate/3-aminoisobutyrate	3-hydroxyisobutyrate		
2	-0.20	1.71		1.25	0.19	0.48	0.46	-0.02		-0.40	0.70	0.44	0.12	-1.08		0.63	1.00	-0.26	0.28	-0.26		-0.01	0.55	0.31	
3	0.31	-0.65	-0.80	0.44	-0.14	-0.61	0.01	-0.16	-0.48	0.19	0.05	-0.65	-0.26	0.10	-1.13	-0.05	-0.17	0.66	0.08	0.30	-0.29	0.38	0.03	-0.11	
4	-0.12	-0.24	-1.29	1.06		-0.50	0.40	-0.58	0.30	-0.28		0.34	0.67	0.10	0.87	-0.28		-0.26	0.53	-0.12	0.63	-0.27		0.01	
5	1.58	-2.00	0.16	-0.19	-0.23	-1.65	0.14	-0.13	0.19	-0.23	-0.51	-0.28	0.48	-0.23	0.26	-0.50	-0.62	-0.26	0.15	0.12	0.09	-0.56	-0.56	-0.05	
6		0.47	0.59	0.83	0.08	-0.45		0.10	0.22	-0.05	-0.02	-0.03		-0.16	-0.12	0.13	-0.03	0.03		0.18	-0.15	0.05	-0.02	0.23	
7	1.18		1.38	-0.04	-1.04	-1.89	0.28		-0.77	0.30	-0.33	0.63	-0.05		-0.84	-0.23	-0.37	0.12	-0.29		-0.19	0.25	-0.39	0.57	
8	0.26	0.47	0.79	0.30	0.04	-1.05	0.11	0.05	0.76	-1.07	0.74	-0.97	0.29	0.01	0.51	-0.36	0.43	-0.66	0.10	-0.21	0.45	0.05	0.11	-0.65	
9	-1.37	0.69	0.01	0.04	1.84	-0.12	-0.30	0.40	-0.34	-0.06	-0.18	-0.06	0.05	0.58	-0.56	0.78	0.35	-0.38	-0.11	0.53	-0.25	0.31	0.11	0.22	
10		-0.77	0.24	0.18	-1.76	0.60		0.71	-0.72	-0.01	0.69	0.00		0.69	-0.51	-0.30	0.24	0.14		0.59	-0.50	0.08	0.43	-0.02	
11	0.07	1.21	-0.16	-0.03	0.32	-0.68	-0.15	0.54	-0.34	-0.30	-0.34	0.05	0.30	-0.79	0.04	-0.66	-0.05	0.27	-0.16	-0.02	-0.46	-0.71	-0.26	0.08	
12	-0.41	0.35	-0.33	-0.48	-1.29	0.51	0.19	0.02	-0.16	0.56	-0.05	-0.21	0.03	-0.60	0.32	-0.14	0.40	-0.61	0.34	-0.30	-0.07	0.19	0.21	-0.20	
13	-1.56	1.14	0.09	-0.19	-1.74	1.52	-0.57	0.01	0.23	-0.10	-0.07	-0.08	-0.82	0.18	0.52	-0.15	-0.64	-0.65	-0.29	0.07	0.35	0.05	-0.09	0.07	
14	0.47	-1.95		1.71	0.04	-1.43	-0.20	-0.53		0.30	-0.89	-0.49	0.32	-0.40		0.56	-0.98	-1.00	0.01	-0.30		0.17	-0.16	-0.62	
15	-1.60	0.65	-1.38	-0.17	-1.39	0.52	-0.13	0.25	-0.02	-0.44	0.17	-0.41	-0.44	0.18	0.28	-0.17	0.22	-0.44	0.01	0.07	0.09	-0.27	0.34	-0.30	
16	-0.10	0.39			-0.47	-0.56	-0.60	0.02			-0.45	-0.58	-0.55	-0.49			0.19	-0.38	-0.50	-0.56		0.01	-0.37		
17	-0.33	-0.11	1.74		0.21	0.21	0.55	-0.39	-0.26		-0.43	0.13	0.95	0.19	0.55		0.15	-0.48	0.20	-0.20	-0.19		-0.40	-0.22	
18	-0.93	-0.48	0.05	-0.60	-0.51	-0.51	-0.24	-0.78	-0.48	-0.43	-0.06	-0.53	0.21	-0.86	-0.72	-1.28	-0.38	-0.08	0.29	-0.32	-0.15	-0.47	-0.29	-0.25	
19		0.98		-1.73	1.07	-1.86		0.16		-1.22	0.29	0.20		0.52		-0.38	-0.17	-0.01		0.22		-0.63	-0.20	0.18	
20	0.72	-0.79	-0.50	0.36	-0.79	-1.74	-0.20	-0.13	-0.46	-0.50	0.44	-0.17	-0.74	-0.21	-0.60	-0.45	0.49	-0.74	-0.22	-0.03	-0.42	-0.28	0.35	-0.18	
	2-hydroxyisobutyrate					3-aminoisobutyrate					3-hydroxybutyrate/3-aminoisobutyrate					3-hydroxyisobutyrate					2-hydroxyisobutyrate				
1	-0.02			0.16	0.23	-0.21	0.30	-0.11		0.90	0.42	0.70	0.21		0.16		-0.20	0.22	-0.01	0.20	-0.05	-0.08	-0.43	0.06	0.60
2	-0.13	0.20		0.34	0.54	0.11	0.19	-0.83		-0.16	0.87	0.50	0.38	-1.00		0.54	0.32	0.04	0.09	0.16		-0.06	0.57	-0.02	
3	-0.14	-0.37	-0.31	0.14	-0.33	0.13	-0.58	-1.07	-0.61	2.00	-0.07	-1.50	0.15	0.28	0.15	0.24	-0.09	-0.46	-0.18	-0.11	0.02	0.19	-0.10	-0.35	
4	0.24	0.09	0.13	0.57		-0.37	0.17	-0.18	-0.06	-0.03		-0.01	0.60	-0.55	0.25	-0.02		-0.65	0.00	0.22	0.72	-0.29		0.33	
5	0.35	-0.27	0.01	-0.13	-0.29	-0.02	1.23	2.00	-0.68	-0.44	-1.05	0.33	-0.11	-0.39	-0.36	-0.79	-0.08	-0.53	0.09	0.08	0.03	-0.69	-0.65	-0.35	
6		0.04	-0.13	-0.17	0.15	-0.11		0.83	-0.35	-1.27	0.13	0.17		0.37	-0.35	0.06	-0.01	0.48		0.19	-0.15	0.09	0.02	0.20	
7	-0.23		-0.24	-0.05	-0.24	-0.17	0.15		-0.65	1.18	0.60	-0.39	-0.44		-0.22	0.13	-0.04	0.02	-0.36		-0.17	-0.15	-0.60	0.19	
8	-0.74	-0.10	0.42	0.23	0.00	-0.30	-2.00	-1.96	-0.65	0.02	0.72	-1.72	-0.27	-0.36	0.16	0.14	-0.16	-0.60	0.05	-0.43	0.30	-0.23	0.34	-0.63	
9	0.15	-0.18	0.18	0.13	0.22	-0.34	-2.00	1.17	-1.10	N	-0.62	0.64	-0.78	0.49	-0.17	-0.18	0.02	-0.01	-0.21	0.58	-0.67	0.10	-0.25	0.07	

		3-hydroxyisovalerate					3-indoxylsulfate					4-deoxyerythronic acid					4-deoxythreonic acid								
10		0.36	0.23	0.10	-0.04	0.20		0.94	-0.15	-0.29	-0.25	0.27		0.28	-0.31	0.81	-0.32	-0.01		0.38	-0.71	0.46	0.38	-0.04	
11		-0.33	0.49	-0.07	0.13	0.15	0.09	-0.13	-0.38	-0.93	-0.13	-0.20	-0.22	0.06	0.09	-0.20	-0.34	-0.24	0.00	0.40	-0.10	-0.04	-0.47	-0.27	0.29
12		0.01	-0.46	0.43	0.29	-0.19	0.23	0.78	-1.18	-1.66	1.87	-0.23	0.67	0.23	-0.75	0.17	-0.49	-0.09	-0.10	0.65	-0.40	-0.22	0.00	0.13	0.26
13		0.32	-0.21	-0.02	-0.21	-0.40	0.18	-0.17	-0.06	-0.42	-0.01	-1.10	0.14	-0.25	0.00	-0.12	0.18	-0.27	-0.05	-0.30	0.09	0.11	-0.07	0.02	-0.33
14		-0.14	0.01		-0.28	0.06	-0.09	-0.51	-0.71		-0.55	-0.63	1.04	-0.28	-0.25		0.25	-0.39	-0.34	0.48	-0.45		-0.25	-0.61	-0.83
15		-0.24	0.22	-0.38	0.58	-0.13	0.20	0.45	-2.00	-0.68	2.00	-1.55	1.07	0.07	-0.54	0.00	-0.72	0.51	0.13	-0.12	-0.36	-0.03	-0.12	0.36	-0.74
16		-0.36	0.11			0.00	0.10	2.00	2.00			0.44	-0.79	-0.69	-0.40			-0.10	-0.19	-0.10	-0.41		0.12	0.12	-0.44
17		0.52	0.29	0.46		-0.35	0.35	2.00	-0.04	-2.00		-1.41	1.23	0.05	0.16	0.36		0.03	0.10	0.08	-0.15	-0.19		-0.41	-0.09
18		-0.12	0.07	-0.22	-0.01	0.07	-0.37	2.00	1.15	-0.14	0.46	2.00	-0.59	0.42	-0.41	-0.03	-0.76	0.12	-0.28	-0.07	-0.71	-0.19	-0.70	-0.99	-0.38
19			-0.13		0.05	-0.01	-0.09		-1.01		-0.26	2.00	0.87		0.38		-0.71	-0.04	0.25		-0.43		-1.24	-0.21	0.17
20		0.37	0.40	0.30	-0.23	0.80	-0.21	0.34	0.29	0.74	0.47	0.07	1.01	0.24	-0.30	-0.21	-0.89	-0.19	-0.30	-0.28	-0.34	-0.87	-0.65	0.07	-0.14
		3-hydroxyisovalerate					3-indoxylsulfate					4-deoxyerythronic acid					4-deoxythreonic acid								
1		0.01		0.02	-0.20	0.59	0.23	0.92		-0.24	1.04	-0.43	0.50	0.15		0.10	0.06	0.42	0.31	0.20		0.35	0.56	0.38	0.29
2		0.26	-0.10		0.43	0.45	0.44	-0.23	-0.21		0.50	0.57	0.03	0.04	-0.17		0.42	0.78	0.33	-0.26	0.38		0.73	0.54	-0.36
3		-0.35	0.00	0.00	0.30	0.05	0.09	-0.39	1.18	-1.32	0.45	-0.10	0.09	-0.04	0.53	-0.17	0.17	0.49	-0.31	0.12	-0.01	0.55	0.09	0.13	0.25
4		0.34	0.45	0.73	-0.16		0.24	-0.71	-0.07	-0.09	0.31		0.20	1.05	0.26	1.04	-0.19		-0.77	0.35	0.65	0.59	0.55		-0.55
5		0.17	-0.21	0.00	-0.32	-0.25	-0.17	0.18	-1.07	0.16	2.00	-1.99	-0.18	0.33	-0.08	-0.12	-0.01	0.08	0.16	0.47	0.88	-0.45	-0.83	0.60	-0.10
6		0.29	-0.32	0.00	0.09	0.15		0.00	1.32	-0.61	2.00	-0.21			0.37	0.44	0.19	0.17	0.33		0.39	0.07	0.14	0.56	0.19
7		0.29		-0.31	-0.06	-0.48	0.35	0.01		-1.82	0.25	-0.43	-0.78	-0.27		-0.08	0.48	0.30	-0.04	-0.70		0.18	0.21	-0.32	0.01
8		0.13	-0.21	0.46	-0.11	0.53	-0.11	0.65	0.02	0.81	1.73	1.72	-1.37	0.44	-0.39	0.40	1.87	-0.36	-0.50	-0.97	0.10	-0.52	0.68	-0.20	0.01
9		-0.02	0.40	-0.55	0.16	0.27	0.18	-2.00	-0.51	0.28	-0.76	1.49	-2.00	0.12	0.56	-0.09	0.47	0.34	0.18	0.10	-0.28	0.00	-0.13	0.78	0.32
10		0.49	-0.21	0.28	0.51	0.23			0.53	0.01	0.73	2.00	0.59		0.62	-0.29	-0.13	0.27	0.08		0.22	-0.03	0.70	0.05	0.31
11		0.10	-0.28	-0.18	-0.54	-0.28	0.22	-0.52	1.70	-0.61	-0.19	0.14	-0.57	0.56	-0.11	0.08	-0.68	0.26	0.06	0.33	-0.10	0.13	0.22	0.18	0.40
12		0.42	-0.48	-0.16	-0.23	0.20	-0.04	0.09	-0.93	0.66	0.23	0.10	-0.64	0.42	-0.03	0.38	-0.19	0.49	-0.11	0.41	-0.83	0.69	0.08	0.48	0.23
13		-0.15	0.10	0.42	0.19	-0.08	-0.37	-0.16	-0.58	0.12	0.05	-0.40	0.91	0.08	0.44	0.41	0.10	0.09	-0.23	0.59	-0.06	0.41	0.07	-0.55	0.42
14		0.33	-0.50		0.06	-0.68	-0.61	-0.40	-0.95		1.95	-0.69	-2.00	-0.01	0.06		-0.01	-0.37	-0.46	0.63	-0.16		0.20	0.59	0.40
15		-0.26	0.51	-0.20	-0.19	0.10	-0.22	-0.45	0.13	-0.03	0.87	-0.17	-0.51	0.40	0.63	-0.17	0.13	0.67	-0.38	0.04	0.16	-0.32	0.43	0.75	0.33
16		-0.27	-0.18			0.01	-0.29	0.52	0.59			-0.28	-0.49	0.15	-0.43			-0.14	0.13	0.59	-0.43			-0.11	0.13
17		0.14	0.02	0.11		-0.24	-0.01	0.28	0.62	0.08		0.52	0.58	0.11	0.03	0.53		-0.27	-0.13	-0.48	0.54	1.41		0.20	0.92

18	-0.12	-0.39	-0.35	-0.52	-0.40	-0.28	0.02	-0.04	-0.57	0.49	-0.91	1.49	0.39	-0.05	-0.16	-0.25	0.01	0.10	-0.01	0.18	0.21	0.31	1.03	-0.01
19		0.27		-0.53	0.02	0.20		2.00		0.89	0.19	-0.48		0.51		-0.59	0.41	0.57		0.49		0.24	0.44	0.37
20	-0.17	-0.08	-0.52	-0.19	0.29	-0.38	-0.18	-0.15	0.60	1.41	0.56	-1.05	-0.13	0.16	-0.19	-0.23	0.05	0.49	0.32	0.68	0.66	0.33	0.88	0.45